

## Ecotox Report for Case # P-17-0023

### General

<b>CBI:</b> Y <b>Status</b> 11/03/2016 <b>Date:</b> <b>SAT Date:</b> 11/04/2016  <b>Consolidated</b> N <b>PMN:</b> <b>Ecotox</b> [REDACTED] <b>Related Cases:</b> [REDACTED] <b>Health</b> [REDACTED] <b>Related Cases:</b> <b>Submitter:</b> [REDACTED] <b>CAS Number:</b> 1072-53-3 <b>Chemical</b> 1,3,2-Dioxathiolane, <b>Name:</b> 2,2-dioxide <b>Use:</b> Additive for use in lithium ion battery electrolyte formulations. CA 158:41102 describes use of a cyclic sulfate ester to improve high temperature performance and cycle performance of lithium ion batteries. [REDACTED] <b>Trade Name:</b> ESA, DTD <b>PV-max(kg/yr):</b> [REDACTED]	<b>Report Status:</b> Complete <b>CRSS Date:</b> 11/03/2016  <b>SAT</b> [REDACTED] <b>Chair:</b> [REDACTED]  <b>Consolidated Set:</b>          <b>Ecotox Assessor:</b> Placeholder, Legacy
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### Fate Summary Statement

<b>Fate P-17-0023</b> <b>Summary</b> <b>Statement:</b> FATE: Solid with MP = 95-97 °C (M) log Kow = -0.90 (E) S > 10 g/L at 25 °C (E) VP = 4.4E-2 torr at 25 °C (E) BP = 209 °C (E) H = 1.15E-6 (E) log Koc = 0.97 (E) log Fish BCF = 0.50 (3)	
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(E)

log Fish BAF = -0.05 (1) (E)

POTW removal (%) = 0-25 via

possible biodeg

Time for complete ultimate aerobic biodeg = wk

Sorption to soils/sediments = low

Volatilization half-life from a

standard river = 570 hrs

Volatilization half-life from a standard lake

= 260 da

Atmospheric Oxidation Half-life = 120 hr via OH radical

PBT Potential: P3B1

\*CEB FATE: Migration to ground water = rapid

Overall wastewater treatment removal is 0-25% based analogous chemicals.

Sorption to sludge is low based on analogous chemicals.

Air Stripping (Volatilization to air) is low based on analogous chemicals and the estimated vapor pressure.

Removal by biodegradation

in wastewater treatment is negligible to moderate based on analogous chemicals and BIOWIN model estimates.

The aerobic aquatic

biodegradation half-life is weeks based on analogous chemicals.

The

anaerobic aquatic biodegradation half-life is months to greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater or equal to the aerobic biodegradation half-life.

Sorption to soil and

sediment is low based on PCKOC model estimates and analogous chemicals.

Migration to groundwater is rapid based on the estimated water solubility and analogous chemicals.

PMN Material:

High Persistence

(P3) is based on the anaerobic biodegradation half-life.

Low

Bioaccumulation potential (B1) is based on analogous chemicals.

## Physical Chemical Information

<b>Molecular Weight:</b>	124.12	
<b>Wt% &lt; 500:</b>		<b>Wt% &lt; 1000:</b>
<b>Physical State - Neat:</b>	Solid	
<b>Melting Point:</b>	95.00 - 97.00	<b>Melting Point (est):</b>
<b>MP (EPI):</b>	95.00	
<b>Vapor Pressure:</b>		<b>Vapor Pressure (est):</b>
<b>VP (EPI):</b>	4.41e-002	0.043
<b>Water Solubility:</b>		<b>Water Solubility (est):</b>
<b>Water Solubility (EPI):</b>		407
<b>Henry's Law::</b>		
<b>Log Koc:</b>		<b>Log Koc (EPI):</b>
<b>Log Kow:</b>		<b>Log Kow (EPI):</b>
<b>Log Kow Comment:</b>		-0.90

## SAT

### Concern Level

<b>Ecotox Rating (1):</b>	2
<b>Ecotox Rating Comment (1):</b>	
<b>Ecotox Rating (2):</b>	
<b>Ecotox Rating Comment (2):</b>	
<b>Ecotox Route of Exposure:</b>	All releases to water

### Ecotox Comments

N
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**Exposure  
Based Review  
(Eco):  
Ecotox  
Comments:  
Exposure Based  
Testing:**

### PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
3	1	2	

### Eco-Toxicity Comment:

### Fate Ratings

Removal0-25 in WWT/POTW (Overall): Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
<b>Fish BCF:</b>						
<b>Log Fish BCF:</b>						
<b>WWT/POTW Sorption:</b>	1	Low	Moderate	Strong	V. Strong	
<b>WWT/POTW Stripping:</b>	3	Extensive	Moderate	Low	Negligible	
<b>Biodegradation Removal:</b>	3-4	Unknown	High	Moderate	Negligible	
<b>Biodegradation Destruction:</b>		Unknown	Complete	Partial	—	
<b>Aerobic Biodeg Ult:</b>	2	<= Days	Weeks	Months	> Months	
<b>Aerobic Biodeg Prim:</b>		<= Days	Weeks	Months	> Months	
<b>Anaerobic Biodeg Ult:</b>	3-4	<= Days	Weeks	Months	> Months	
<b>Anaerobic Biodeg Prim:</b>		<= Days	Weeks	Months	> Months	
<b>Hydrolysis (t1/2 at pH 7,25C) A:</b>		<= Minutes	Hours	Days	>= Months	

Removal0-25 in WWT/POTW (Overall):						
Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	4	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	4	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	
<b>Bio Comments:</b> Overall wastewater treatment removal is 0-25% based analogous chemicals. Sorption to sludge is low based on analogous chemicals. Air Stripping (Volatilization to air) is low based on analogous chemicals and the estimated vapor pressure. Removal by biodegradation in wastewater treatment is negligible to moderate based on analogous chemicals and BIOWIN model estimates. The aerobic aquatic biodegradation half-life is weeks based on analogous chemicals. The anaerobic aquatic biodegradation half-life is months to greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater or equal to the aerobic biodegradation half-life. Sorption to soil and sediment is low based on PCKOC model estimates and analogous chemicals.  Migration to groundwater is rapid based on the estimated water solubility and analogous chemicals. PMN Material: High Persistence (P3) is based on the anaerobic biodegradation half-life. Low						

Removal0-25 in WWT/POTW (Overall):					Comment
Condition	Rating Values	1	2	Rating Description 3	
				4	
<p>Bioaccumulation potential (B1) is based on analogous chemicals.</p> <p><b>Fate</b> Overall wastewater treatment</p> <p><b>Comments:</b> removal is 0-25% based analogous chemicals.</p> <p>Sorption to sludge is low based on analogous chemicals.</p> <p>Air Stripping (Volatilization to air) is low based on analogous chemicals and the estimated vapor pressure.</p> <p>Removal by biodegradation in wastewater treatment is negligible to moderate based on analogous chemicals and BIOWIN model estimates. The aerobic aquatic biodegradation half-life is weeks based on analogous chemicals. The anaerobic aquatic biodegradation half-life is months to greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater or equal to the aerobic biodegradation half-life.</p> <p>Sorption to soil and sediment is low based on PCKOC model estimates and analogous chemicals.</p> <p>Migration to groundwater is rapid based on the estimated water solubility and analogous chemicals.</p> <p>PMN Material: High Persistence (P3) is based on the anaerobic biodegradation half-life.</p> <p>Low Bioaccumulation potential (B1) is based on analogous chemicals.</p>					

### Ecotoxicity Values

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
<b>Fish</b>	96-h	LC50	>100	>15.2	
<b>Daphnid</b>	48-h	LC50	>100		
<b>Green Algae</b>	96-h	EC50	>100	>9.1	
<b>Fish</b>	-	Chronic Value	>10		
<b>Daphnid</b>	-	Chronic Value	>10		
<b>Green Algae</b>	-	Chronic Value	>10	5	

Test organism	Test Type	Test Endpoint	Predicted	Experimental Comments
Ecotox Value	Predictions are based on SARs for esters; SAR			
Comments:	chemical class = ester; MW 124; solid with mp = 97 C (M); S = 38.2 g/L at 20 C (P); pH7; effective concentrations based on 100% active ingredients and nominal concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L;			
<p>Acute base set toxicity testing was submitted with a [REDACTED]. The testing used an acceptable study method, but the testing did not test to high enough concentrations resulting in non-definitive (i.e., &gt;) EC/LC50 values (see reviews below). However, the algae test did yield a definitive ChV. This ChV was used to derive the acute and chronic concentrations of concern for P-17-0023.</p> <p>Focus Report/Decision Document: Environmental Hazard and Risk (P-17-0023)</p> <p>Environmental Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risks because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model (<a href="https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model">https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model</a>) and hazard data for the new chemical substance. Based on these estimated hazard values from ECOSAR and hazard values from test data for the new chemical substance, EPA concludes that this chemical substance has moderate environmental hazard.</p> <ul style="list-style-type: none"><li>· Substance falls within the TSCA New Chemicals Category of Esters.</li><li>· ECOSAR chemical class of esters.</li><li>· Acute base set toxicity testing (fish, daphnid, algae) was submitted with a [REDACTED]. The testing used an acceptable study method, but the testing did not test to high enough concentrations resulting in non-definitive (i.e., &gt;) EC/LC50 values. However, the algae test did yield a definitive chronic value (ChV). This ChV was used to derive the acute and chronic concentrations of concern for P-17-0023.</li><li>· Moderate hazard based on acute and chronic concentrations of concern of 5,000 ppb</li></ul>				

Test organism	Test Type	Test Endpoint	Predicted	Experimental Comments
				<p>and 500 ppb, respectively.</p> <p>Environmental Risk:</p> <ul style="list-style-type: none"> <li>· Risks were not identified for ecotoxicity.</li> </ul> <p>Testing Recommendations:</p> <ul style="list-style-type: none"> <li>· No testing is recommended.</li> </ul> <p>Data from same as [REDACTED]</p> <p>Fish</p> <p>Ecotoxicity Test:</p> <div style="background-color: black; width: 100%; height: 500px; position: relative;"> <div style="position: absolute; bottom: 20px; right: 20px; background-color: white; padding: 5px;">This study is acceptable.</div> </div>



Test organism	Test Type	Test Endpoint	Predicted	Experimental Comments
		96-hr LC50 > 15.238 mg/L		Daphnid Ecotoxicity Test:
				[REDACTED]
				This study is acceptable.
		48-hour EC50 > 12.429 mg/L		Algal Ecotoxicity Test:
				[REDACTED]

[illegible]

Test organism	Test Type	Test Endpoint	Predicted	Experimental Comments
	72-hour LOEC (growth rate) = 5.59 mg/L 72-hour ChV (growth rate) = 4.98 mg/L			
				The acute base-set (aquatic fish, aquatic invertebrate, and aquatic plant) studies are acceptable.
				However, dose ranges for this test substance is inadequate. Therefore, the predicted values will be used to assess the ecotoxicity of [REDACTED]. Predictions based on SAR analysis for esters are >100 mg/L for the acute fish, daphnia, and green algae endpoints, and >10 mg/L for the chronic fish, daphnia, and green algae endpoints. The acute CoC for [REDACTED] is determined from the predicted 96-hour LC50 fish toxicity study of >100 mg/L. The acute CoC is derived by dividing the 96-hour green algal LC50 of >100 mg/L (1,000 ppb) by an assessment factor of 5 yielding an acute CoC of 20,000 ppb. The chronic CoC is derived by dividing the predicted chronic fish toxicity value of 10 mg/L by an uncertainty factor of 10, yielding 10 mg/L or 1,000 ppb.
				Ecotox Study Reviewer: [REDACTED] [REDACTED]

### Ecotox Factors

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic (ppb):		4/10	5000	
Chronic Aquatic (ppb):			500	

Factors	Values	Comments
SARs: esters		
SAR esters		
Class:		
TSCA		
NCC Category?	Esters	

Recommended Testing:
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<b>Ecotox Factors Comments:</b>
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**Comments/Telephone Log**

Artifact	Update/Upload Time
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